Inclusion of Diffraction Effects in the Gutzwiller Trace Formula

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Abstract - The Gutzwiller trace formula is extended to include diffraction effects. The new trace formula involves periodic rays which have non-geometrical segments as a result of diffraction on the surfaces and edges of the scatter.

Gutzwiller's trace formula[1] is an increasingly popular tool for analyzing semiclassical behaviour. Recently, it has been demonstrated that using proper mathematical apparatus, like Gutzwiller-Voros[2] zeta functions, cycle expansions[3] or quantum Fredholm determinants[4], the trace formula can successfully predict individual eigenenergies of bound systems and resonances of open scattering systems. The physical content of the trace formula is the geometrical optical approximation of quantum mechanics via canonical invariants of closed classical orbits. This approximation is very accurate when periodic orbits sufficiently cover the phase space of the chaotic system. This is not the case when the number of obstacles is small or their distance is large compared to their typical size. Such a problem occurs where the wave length of a quantum mechanical (or optical) wave is very large compared to the spatial variation of a repulsive potential, e.g. at the boundaries of microwave guides, optical fibers, superconducting squids, or circuits in the ballistic electron transport, i.e. in most of the devices used for so-called macroscopic quantum mechanical (or optical) experiments. In such cases it is important to take into account the next-to-geometrical effects. In Ref. 5 we have shown how the *Geometric Theory of Diffraction* (GTD) for hard core potentials can be incorporated in the periodic orbit theory. (Since the space here is limited, we invite the reader to study reference 5 for more details and explicite formulas.)

The diffracted rays connecting two points in the configuration space can be derived from an extension of Fermat's variational principle of classical mechanics[6]. The generalized principle requires new classes of curves: We have to consider for each triplet of integers $r, s, t \geq 0$ the class of curves $\mathcal{D}_{rst}$ with r smooth arcs on the surface, s points on the edges and t points on the vertices of the boundary or the discontinuity. The curves of the GTD are those which make the classical action stationary within one of the classes $\mathcal{D}_{rst}$. The class $\mathcal{D}_{000}$ corresponds to the usual geometrical orbits. Once we know the generalized ray connecting $\mathcal{A}$ and $\mathcal{B}$ we can compute semiclassically the Green's function $G(q_{\mathcal{A}}, q_{\mathcal{B}}, E)$ by tracing the ray[6]:

a, On the geometrical segments of the ray, the Green's function is given by the energy domain Van-Vleck propagator

$$G(q, q', E) = \frac{2\pi}{(2\pi i\hbar)^{3/2}} D_{\mathrm{V}}^{1/2}(q, q', E) e^{\frac{i}{\hbar}S(q,q',E) - \frac{i}{2}\nu\pi}, \tag{1}$$

where $D_{\mathrm{V}}(q, q', E) = |\det(-\partial^2 S/\partial q_i \partial q'_j)|/|\dot{q}||\dot{q}'|$ is the Van-Vleck determinant and ν is the Maslov index.

b, When the geometrical ray hits a surface, an edge or a vertex of the obstacle it creates a source for the diffracted wave. The strength of the source is proportional to the Green's function at the incidence of the ray

$$Q_{\mathrm{diff}} = D G_{\mathrm{inci}} \,. \tag{2}$$

The diffraction constant D depends on the local geometry and the nature of the diffraction. It has been determined in Ref. 6 from the asymptotic semiclassical expansion of the exact solution in a simple geometry[6,7]. For the surface diffraction (creeping) its form is

$$D_l = 2^{1/3} 3^{-2/3} \pi e^{5i\pi/12} \frac{(k\rho)^{1/6}}{Ai'(x_l)} \,. \tag{3}$$

Here $Ai'(x)$ is the derivative of the Airy function, $k = \sqrt{2mE/\hbar}$ is the wave number, ρ is the radius of the obstacle at the source of the creeping ray and x_l are the zeroes of the Airy integral. The index $l \geq 1$ refers to the possibility of initiating creeping rays with different modes, each with its own profile. In practice only the low modes contribute to the Green's function. For edge diffraction the diffraction constant is

$$D = \frac{\sin(\pi/n)}{n} \left[(\cos(\pi/n) - \cos((\theta - \alpha)/n))^{-1} - (\cos(\pi/n) - \cos((\theta + \alpha + \pi)/n))^{-1} \right], \tag{4}$$

where $(2-n)\pi$ is the angle of the edge (n is a real number), α is the incident angle and θ is the outgoing angle. For details we refer to Ref. 6. The source then initiates a ray propagating along the surface (for creeping) or a ray starting at the edge of the obstacle (edge diffraction). When the creeping ray leaves the surface its intensity can be calculated from the relation (2) due to the reversibility of the Green's function. The total Green's function is then the *product* of the Green's functions and diffraction coefficients along the ray. If for example we have geometrical propagation from $\mathcal{A}$ to $\mathcal{A}'$, then a surface creeping from $\mathcal{A}'$ to $\mathcal{B}'$ and then again a geometrical propagation from $\mathcal{B}'$ to $\mathcal{B}$, the total semiclassical Green's function is

$$G(q_{\mathcal{A}}, q_{\mathcal{B}}, E) = G(q_{\mathcal{A}}, q_{\mathcal{A}'}, E) D_{\mathcal{A}'} G^{\mathrm{creeping}}(q_{\mathcal{A}'}, q_{\mathcal{B}'}, E) D_{\mathcal{B}'} G(q_{\mathcal{B}'}, q_{\mathcal{B}}, E). \tag{5}$$

Contrary to the pure geometrical case the semiclassical energy-domain Green's function for rays with diffraction arcs have a multiplicative composition law. When we incorporate diffraction effects into the trace formula, periodic rays with diffraction segments also contribute. We can handle separately the pure geometric cycles and the cycles with at least one diffraction arc or edge:

$$\mathrm{Tr}\, G(E) \approx \mathrm{Tr}\, G_G(E) + \mathrm{Tr}\, G_D(E), \tag{6}$$

where $\mathrm{Tr}\, G_G(E)$ is the ordinary Gutzwiller trace formula, while $\mathrm{Tr}\, G_D(E)$ is the new trace formula corresponding to the non-trivial cycles of the GTD. $\mathrm{Tr}\, G_D(E)$ can be computed by using appropriate Watson contour integrals[7]. For technical details we refer the reader to Refs. 5 and 8. If we denote by q_i, $i = 1, \ldots, n$ (with $q_{n+i} \equiv q_i$) the points along the closed cycle, where the ray changes from diffraction to pure geometric evolution or vice versa the trace for cycles with *at least one diffraction arc* can be expressed as the product

$$\mathrm{Tr}\, G_D(E) = \frac{1}{i\hbar} \sum_{\text{Cycles}} T(E) \prod_{i=1}^{n} D(q_i) G(q_i, q_{i+1}, E), \tag{7}$$

where $T(E)$ is the time period of the primitive cycle and $D(q_i)$ is the diffraction constant (3) at the point q_i. $G(q_i, q_{i+1}, E)$ is alternatingly the Van-Vleck propagator, if q_i and q_{i+1} are connected by pure geometric arcs, or is given by creeping propagator[7] in case q_i and q_{i+1} are the boundary points of a creeping arc. The cycles with diffractional parts have the special property that their energy domain Green's functions are *multiplicative* along the ray. This does not hold for pure geometrical cycles.

The eigenenergies can be recovered from the Gutzwiller-Voros spectral determinant[2] $\Delta(E)$, which is related to the trace formula as

$$\mathrm{Tr}\, G(E) = \frac{d}{dE} \ln \Delta(E). \tag{8}$$

The full semiclassical determinant can be written as the formal product of two spectral determinants, one corresponding to pure geometrical cycles and one to the new diffraction cycles, $\Delta(E) = \Delta_G(E)\Delta_D(E)$ due to the additivity of the traces. The diffraction part of the spectral determinant is

$$\Delta_D(E) = \exp\left(- \sum_{p,r=1}^{\infty} \frac{1}{r} \prod_{i=1}^{n_p} [D(q_i^p) G(q_i^p, q_{i+1}^p, E)]^r \right), \tag{9}$$

where the summation goes over closed primitive cycles p and the repetition number r.

To demonstrate the importance of the diffraction effects to the spectra, we have calculated the resonances of the scattering system of two equally sized hard circular disks[5,8]. This system has a C_{2v} symmetry with four one-dimensional irreducible representations. In Fig. 1 we show the B_1 resonances. In this system there is only one geometrical unstable cycle along the line connecting the centers of the disks. In Fig. 1 we see that the new formula describes the leading resonances with a few percent error, while the computation based on the geometrical cycle alone would give completely false result.

Figure 1: B_1 Resonances of the two-disk system[5,8] with disk separation $R = 6a$ in the complex k plane in units of the inverse disk radius a. The diamonds label the exact resonances, the crosses are their semiclassical approximations from the new extended trace formula. These resonances cannot be predicted from the Gutzwiller trace formula.

In bound systems the edge diffraction is probably more important than the creeping diffraction. Recently, in Ref. 9, an edge diffraction cycle has been observed in the Fourier transformed level density. The amplitude of such a diffraction term can be calculated from (7) using the diffraction constant (4).

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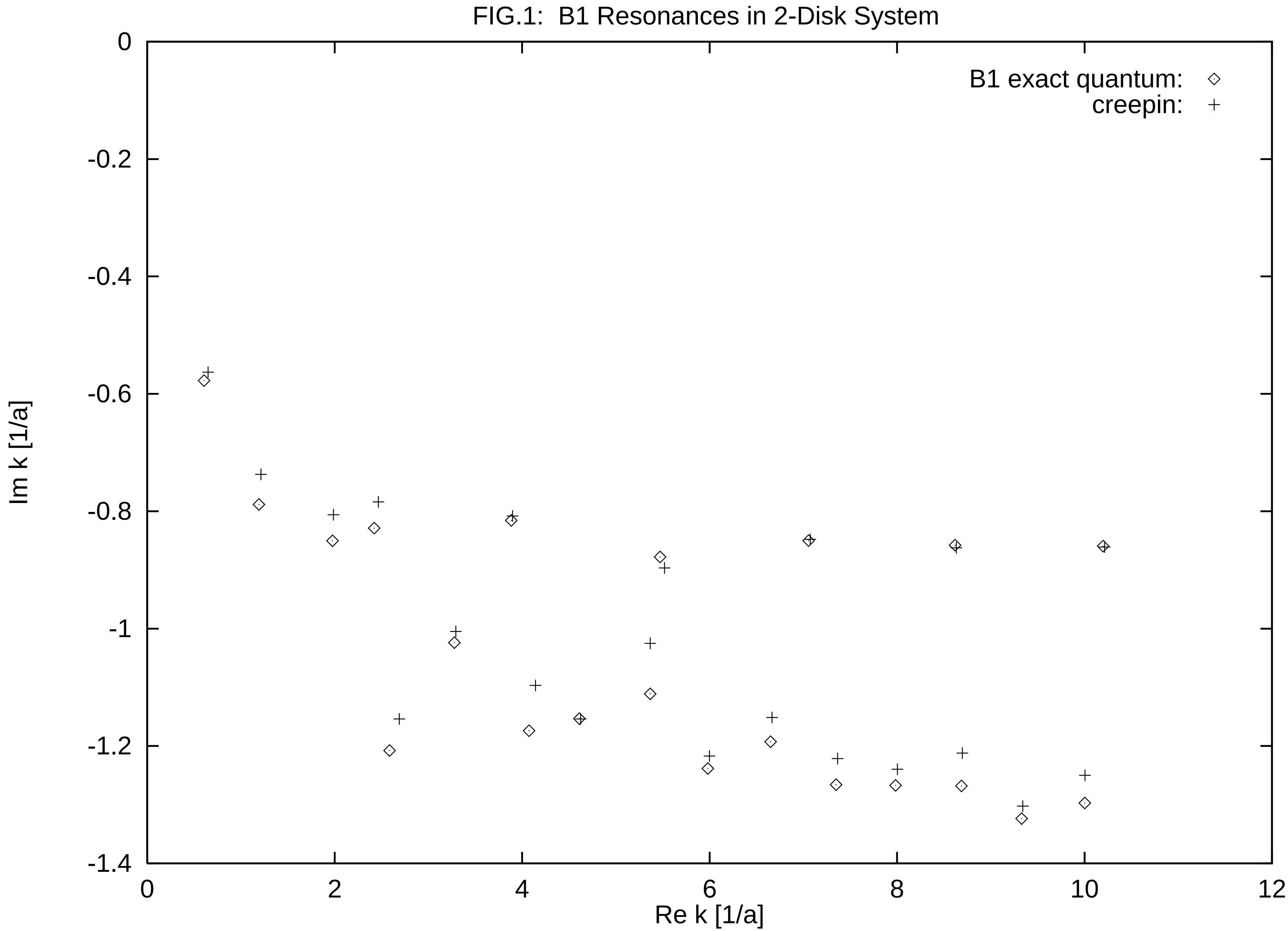
FIG.1: B1 Resonances in 2-Disk System
B1 exact quantum:
creepin:
Im k [1/a]
Re k [1/a]
0
-0.2
-0.4
-0.6
-0.8
-1
-1.2
-1.4
0
2
4
6
8
10
12